



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:11 am GMT

PDB ID : 2QIZ
Title : Structure of the yeast U-box-containing ubiquitin ligase Ufd2p
Authors : Tu, D.; Brunger, A.T.
Deposited on : 2007-07-06
Resolution : 2.56 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

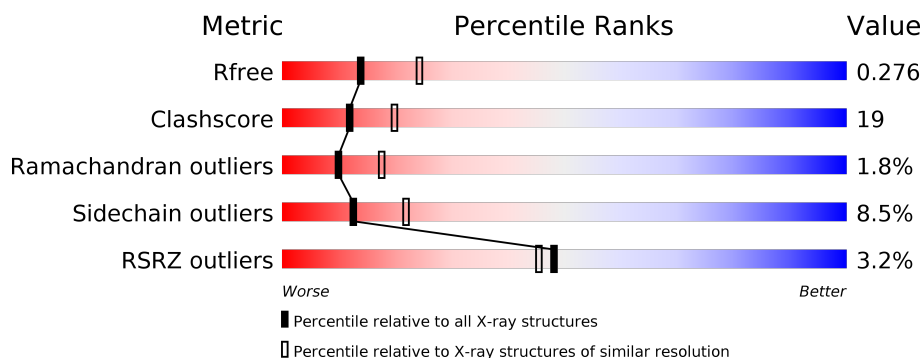
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3689 (2.60-2.52)
Clashscore	112137	4096 (2.60-2.52)
Ramachandran outliers	110173	4037 (2.60-2.52)
Sidechain outliers	110143	4037 (2.60-2.52)
RSRZ outliers	101464	3700 (2.60-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	982	<div> <div>3%</div> <div>59%</div> <div>32%</div> <div>5%</div> <div>.</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7767 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ubiquitin conjugation factor E4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	943	Total	C	N	O	S	0	0	0
			7621	4896	1255	1442	28			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	GLY	-	EXPRESSION TAG	UNP P54860
A	-19	SER	-	EXPRESSION TAG	UNP P54860
A	-18	HIS	-	EXPRESSION TAG	UNP P54860
A	-17	MET	-	EXPRESSION TAG	UNP P54860
A	-16	ALA	-	EXPRESSION TAG	UNP P54860
A	-15	SER	-	EXPRESSION TAG	UNP P54860
A	-14	MET	-	EXPRESSION TAG	UNP P54860
A	-13	THR	-	EXPRESSION TAG	UNP P54860
A	-12	GLY	-	EXPRESSION TAG	UNP P54860
A	-11	GLY	-	EXPRESSION TAG	UNP P54860
A	-10	GLN	-	EXPRESSION TAG	UNP P54860
A	-9	GLN	-	EXPRESSION TAG	UNP P54860
A	-8	MET	-	EXPRESSION TAG	UNP P54860
A	-7	GLY	-	EXPRESSION TAG	UNP P54860
A	-6	ARG	-	EXPRESSION TAG	UNP P54860
A	-5	GLY	-	EXPRESSION TAG	UNP P54860
A	-4	SER	-	EXPRESSION TAG	UNP P54860
A	-3	GLU	-	EXPRESSION TAG	UNP P54860
A	-2	PHE	-	EXPRESSION TAG	UNP P54860
A	-1	ARG	-	EXPRESSION TAG	UNP P54860
A	0	SER	-	EXPRESSION TAG	UNP P54860
A	102	LEU	SER	ENGINEERED	UNP P54860
A	677	VAL	ASP	ENGINEERED	UNP P54860

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	K 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total 145	O 145	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.50Å 122.99Å 176.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.56 44.83 – 2.56	Depositor EDS
% Data completeness (in resolution range)	93.6 (50.00-2.56) 92.6 (44.83-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.54Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.221 , 0.276 0.221 , 0.276	Depositor DCC
R_{free} test set	4370 reflections (10.05%)	DCC
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7767	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
K

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/7781	0.58	0/10515

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7621	0	7597	292	0
2	A	1	0	0	0	0
3	A	145	0	0	5	0
All	All	7767	0	7597	292	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (292) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ILE:H	1:A:114:ILE:HD12	1.12	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:SER:HB2	1:A:851:PRO:HA	1.45	0.99
1:A:207:LYS:HB3	1:A:209:GLN:NE2	1.79	0.95
1:A:926:ARG:HH11	1:A:926:ARG:HB2	1.28	0.94
1:A:293:ASN:HD21	1:A:307:SER:H	0.98	0.93
1:A:576:HIS:HB2	1:A:633:GLN:NE2	1.84	0.92
1:A:207:LYS:HB3	1:A:209:GLN:HE22	1.35	0.92
1:A:842:LEU:HB3	1:A:848:LEU:HD13	1.52	0.91
1:A:125:ASN:O	1:A:128:THR:HG22	1.70	0.90
1:A:630:SER:HB2	1:A:633:GLN:HB3	1.54	0.87
1:A:494:GLN:HE21	1:A:495:ILE:H	1.19	0.86
1:A:209:GLN:HG2	1:A:304:LYS:O	1.80	0.82
1:A:567:ARG:HG3	1:A:613:ASN:HB3	1.65	0.78
1:A:293:ASN:HD21	1:A:307:SER:N	1.81	0.78
1:A:566:LEU:HD21	1:A:582:VAL:HG23	1.65	0.76
1:A:876:LEU:HD12	1:A:876:LEU:O	1.86	0.76
1:A:494:GLN:HE21	1:A:495:ILE:N	1.84	0.76
1:A:64:PHE:O	1:A:68:GLN:HG2	1.85	0.76
1:A:68:GLN:HE22	1:A:71:LYS:NZ	1.84	0.75
1:A:657:SER:O	1:A:661:GLN:HG3	1.87	0.75
1:A:215:THR:HG21	1:A:285:TYR:OH	1.85	0.75
1:A:276:LEU:HA	1:A:279:ARG:NH1	2.03	0.73
1:A:852:GLU:O	1:A:855:GLU:HB3	1.88	0.73
1:A:99:VAL:HG22	1:A:134:ILE:HG23	1.70	0.73
1:A:114:ILE:H	1:A:114:ILE:CD1	1.89	0.73
1:A:234:ASN:HB3	1:A:249:ILE:HD12	1.71	0.71
1:A:926:ARG:HB2	1:A:926:ARG:NH1	2.04	0.71
1:A:494:GLN:NE2	1:A:495:ILE:H	1.89	0.71
1:A:147:LEU:O	1:A:151:VAL:HG12	1.90	0.70
1:A:789:VAL:HG23	1:A:792:PRO:HG3	1.71	0.70
1:A:68:GLN:HE22	1:A:71:LYS:HZ2	1.36	0.70
1:A:335:ASP:HB2	3:A:1107:HOH:O	1.89	0.70
1:A:894:MET:HE3	1:A:907:ILE:C	2.12	0.70
1:A:26:GLU:O	1:A:27:GLU:HB2	1.91	0.70
1:A:848:LEU:HG	1:A:850:SER:OG	1.92	0.70
1:A:95:ILE:HD11	1:A:137:ARG:NH1	2.07	0.70
1:A:497:LEU:HD22	1:A:609:LEU:HD11	1.72	0.69
1:A:185:VAL:HG22	1:A:270:LYS:HB3	1.73	0.68
1:A:114:ILE:N	1:A:114:ILE:HD12	1.98	0.68
1:A:404:GLU:HA	1:A:407:MET:HG3	1.76	0.68
1:A:234:ASN:HB3	1:A:249:ILE:CD1	2.24	0.67
1:A:23:LEU:HD23	1:A:23:LEU:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ILE:HB	1:A:392:TYR:OH	1.95	0.67
1:A:898:VAL:HG21	1:A:912:ILE:HD11	1.78	0.66
1:A:721:LYS:HG3	1:A:722:GLU:H	1.60	0.66
1:A:721:LYS:HG3	1:A:722:GLU:N	2.12	0.65
1:A:850:SER:HA	1:A:853:PHE:H	1.62	0.65
1:A:132:SER:O	1:A:136:GLN:HG3	1.96	0.65
1:A:238:ASN:O	1:A:241:ARG:HG2	1.96	0.64
1:A:235:TYR:OH	1:A:250:HIS:HD2	1.79	0.64
1:A:722:GLU:O	1:A:726:ARG:HB2	1.98	0.64
1:A:592:LEU:HD12	1:A:592:LEU:N	2.13	0.64
1:A:117:ILE:HG12	1:A:154:THR:HG22	1.80	0.63
1:A:356:ARG:HG3	1:A:525:TYR:O	1.99	0.63
1:A:848:LEU:HD11	1:A:854:ILE:HD11	1.81	0.63
1:A:556:GLY:O	1:A:560:GLU:HG3	1.98	0.62
1:A:128:THR:HG23	1:A:129:ASP:H	1.64	0.62
1:A:850:SER:HB2	1:A:851:PRO:CA	2.26	0.61
1:A:848:LEU:C	1:A:850:SER:H	2.03	0.61
1:A:837:ARG:HB3	1:A:837:ARG:NH1	2.15	0.61
1:A:833:ASN:O	1:A:837:ARG:HG2	2.01	0.61
1:A:506:VAL:HG11	1:A:675:ARG:HH21	1.65	0.60
1:A:373:LYS:HA	1:A:373:LYS:HZ3	1.65	0.60
1:A:839:VAL:HG22	1:A:854:ILE:HG23	1.84	0.60
1:A:605:GLU:HB2	1:A:655:ILE:HD13	1.84	0.60
1:A:250:HIS:O	1:A:254:GLN:HG3	2.01	0.59
1:A:249:ILE:HG13	1:A:253:LEU:HD22	1.84	0.59
1:A:498:PRO:HG3	1:A:567:ARG:NH1	2.17	0.59
1:A:404:GLU:HB3	1:A:456:LEU:HD13	1.85	0.59
1:A:922:ASP:HB3	1:A:925:ASN:ND2	2.18	0.59
1:A:735:LYS:HA	1:A:795:TYR:O	2.02	0.58
1:A:732:ARG:HB2	1:A:732:ARG:NH1	2.17	0.58
1:A:820:ILE:CD1	1:A:864:ALA:HA	2.33	0.58
1:A:752:SER:O	1:A:756:PRO:HG3	2.03	0.58
1:A:848:LEU:O	1:A:850:SER:N	2.36	0.58
1:A:701:ILE:O	1:A:705:LEU:HG	2.04	0.58
1:A:56:PRO:O	1:A:59:TYR:HB3	2.03	0.58
1:A:789:VAL:CG2	1:A:792:PRO:HG3	2.34	0.57
1:A:915:HIS:CD2	1:A:923:PRO:HG3	2.39	0.57
1:A:77:LYS:HB3	1:A:78:PRO:HD2	1.85	0.57
1:A:261:ILE:HD11	1:A:321:ARG:NH2	2.19	0.57
1:A:494:GLN:HE21	1:A:494:GLN:CA	2.17	0.57
1:A:520:PRO:HG3	1:A:571:LEU:CD2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:PRO:HD2	1:A:941:ARG:HG3	1.87	0.57
1:A:591:PRO:C	1:A:592:LEU:HD12	2.25	0.57
1:A:659:LYS:O	1:A:663:ILE:HG13	2.05	0.57
1:A:83:LEU:HB3	1:A:87:PHE:CE2	2.40	0.57
1:A:925:ASN:C	1:A:925:ASN:HD22	2.07	0.57
1:A:36:VAL:HG22	1:A:86:THR:HG22	1.87	0.56
1:A:180:ILE:O	1:A:180:ILE:HD12	2.05	0.56
1:A:631:SER:O	1:A:632:SER:HB2	2.06	0.56
1:A:727:LEU:C	1:A:727:LEU:HD23	2.26	0.56
1:A:14:PRO:HA	1:A:22:LEU:HD11	1.88	0.56
1:A:68:GLN:NE2	1:A:71:LYS:NZ	2.54	0.55
1:A:521:VAL:HB	1:A:522:PRO:CD	2.36	0.55
1:A:621:PHE:O	1:A:625:VAL:HG22	2.06	0.55
1:A:208:PRO:HG2	1:A:305:GLU:O	2.06	0.55
1:A:521:VAL:HB	1:A:522:PRO:HD3	1.88	0.55
1:A:848:LEU:N	1:A:848:LEU:HD23	2.21	0.55
1:A:724:GLN:NE2	1:A:724:GLN:HA	2.21	0.55
1:A:820:ILE:O	1:A:820:ILE:HD12	2.06	0.55
1:A:293:ASN:ND2	1:A:307:SER:H	1.83	0.55
1:A:135:ILE:O	1:A:139:ILE:HG23	2.06	0.55
1:A:232:ILE:HG13	1:A:233:ARG:N	2.22	0.55
1:A:682:ASN:OD1	1:A:767:ARG:NH2	2.37	0.54
1:A:847:GLY:O	1:A:848:LEU:HB3	2.06	0.54
1:A:217:LEU:HB3	1:A:221:LEU:CD1	2.38	0.54
1:A:105:GLU:OE2	1:A:112:ALA:HB1	2.07	0.54
1:A:772:LEU:HD22	1:A:806:LEU:CD1	2.37	0.54
1:A:485:ASP:HB2	1:A:495:ILE:HD12	1.88	0.54
1:A:398:GLY:HA2	1:A:401:LEU:HD21	1.90	0.54
1:A:22:LEU:HD23	1:A:23:LEU:N	2.23	0.54
1:A:241:ARG:HD2	3:A:997:HOH:O	2.08	0.53
1:A:565:VAL:HG13	1:A:572:VAL:CG1	2.37	0.53
1:A:780:VAL:CG1	1:A:837:ARG:HB2	2.38	0.53
1:A:683:ASP:HA	1:A:686:PHE:CE2	2.43	0.53
1:A:790:LYS:O	1:A:792:PRO:HD3	2.08	0.53
1:A:0:SER:OG	1:A:86:THR:HG21	2.08	0.53
1:A:509:VAL:O	1:A:510:ASP:C	2.47	0.53
1:A:780:VAL:HG13	1:A:837:ARG:HB2	1.89	0.53
1:A:217:LEU:HB3	1:A:221:LEU:HD12	1.90	0.53
1:A:506:VAL:HG22	1:A:627:LYS:NZ	2.24	0.53
1:A:850:SER:HB3	1:A:854:ILE:HG13	1.91	0.53
1:A:117:ILE:C	1:A:117:ILE:HD12	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:916:LEU:HA	1:A:919:ASP:O	2.09	0.52
1:A:642:TYR:CE2	1:A:646:ILE:HD11	2.45	0.52
1:A:40:ASP:HA	1:A:93:LEU:HD13	1.91	0.52
1:A:773:ASN:ND2	1:A:810:TYR:OH	2.42	0.51
1:A:505:GLY:C	1:A:507:GLU:H	2.13	0.51
1:A:207:LYS:CB	1:A:209:GLN:HE22	2.17	0.51
1:A:43:LEU:HD23	1:A:97:TYR:HD2	1.75	0.51
1:A:373:LYS:NZ	1:A:373:LYS:HA	2.25	0.51
1:A:99:VAL:CG2	1:A:134:ILE:HG23	2.38	0.51
1:A:12:THR:HG22	1:A:23:LEU:HD21	1.93	0.51
1:A:74:THR:HG22	1:A:80:ALA:HA	1.93	0.50
1:A:896:ASP:OD1	1:A:909:ARG:HD2	2.11	0.50
1:A:95:ILE:HD11	1:A:137:ARG:HH12	1.75	0.50
1:A:804:LYS:HZ1	1:A:849:ALA:H	1.59	0.50
1:A:3:ALA:HA	3:A:1070:HOH:O	2.12	0.50
1:A:567:ARG:HD3	1:A:567:ARG:O	2.12	0.50
1:A:169:ASN:O	1:A:171:SER:N	2.44	0.50
1:A:173:ILE:O	1:A:177:VAL:HG23	2.12	0.50
1:A:137:ARG:HH11	1:A:137:ARG:HG2	1.77	0.49
1:A:611:ASN:HA	1:A:658:TYR:OH	2.12	0.49
1:A:54:ASP:C	1:A:56:PRO:HD3	2.32	0.49
1:A:754:ASP:C	1:A:756:PRO:HD3	2.33	0.49
1:A:884:GLU:HG3	1:A:885:PHE:CD2	2.47	0.49
1:A:175:ASN:HD22	1:A:263:ARG:NH1	2.10	0.49
1:A:297:ARG:HH11	1:A:297:ARG:CG	2.24	0.49
1:A:565:VAL:HG13	1:A:572:VAL:HG12	1.94	0.49
1:A:729:SER:HA	1:A:732:ARG:NH2	2.27	0.49
1:A:576:HIS:HB2	1:A:633:GLN:HE21	1.71	0.49
1:A:592:LEU:HD13	1:A:596:SER:O	2.12	0.49
1:A:687:LEU:HD11	1:A:740:LEU:HD13	1.94	0.49
1:A:26:GLU:O	1:A:27:GLU:CB	2.59	0.49
1:A:316:THR:OG1	1:A:392:TYR:HB3	2.13	0.49
1:A:702:GLN:HE21	1:A:727:LEU:HD11	1.77	0.49
1:A:175:ASN:HD22	1:A:263:ARG:HH12	1.61	0.48
1:A:506:VAL:HG22	1:A:627:LYS:HZ1	1.76	0.48
1:A:242:SER:OG	1:A:245:GLN:HG3	2.12	0.48
1:A:724:GLN:C	1:A:726:ARG:N	2.67	0.48
1:A:832:ARG:HG2	1:A:832:ARG:HH11	1.77	0.48
1:A:412:LYS:O	1:A:416:GLU:HG3	2.13	0.48
1:A:448:THR:O	1:A:452:LEU:HB2	2.13	0.48
1:A:804:LYS:HZ3	1:A:848:LEU:HA	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLN:CG	1:A:305:GLU:HA	2.43	0.48
1:A:4:ILE:O	1:A:8:LEU:HB2	2.14	0.48
1:A:137:ARG:HH11	1:A:137:ARG:CG	2.26	0.48
1:A:574:ASN:OD1	1:A:576:HIS:HB3	2.14	0.47
1:A:215:THR:CG2	1:A:285:TYR:OH	2.61	0.47
1:A:594:ASP:O	1:A:595:ASN:HB2	2.14	0.47
1:A:780:VAL:HG13	1:A:837:ARG:CB	2.43	0.47
1:A:128:THR:HG23	1:A:129:ASP:N	2.29	0.47
1:A:162:HIS:HE1	3:A:1062:HOH:O	1.97	0.47
1:A:538:SER:HA	1:A:541:ILE:HD11	1.97	0.47
1:A:567:ARG:CG	1:A:613:ASN:HB3	2.43	0.47
1:A:831:ASN:ND2	1:A:833:ASN:HB3	2.30	0.46
1:A:92:ARG:HH12	1:A:93:LEU:HD21	1.80	0.46
1:A:228:ALA:HA	1:A:452:LEU:HD13	1.97	0.46
1:A:621:PHE:HD2	1:A:644:ILE:HD11	1.79	0.46
1:A:894:MET:HE3	1:A:907:ILE:CA	2.44	0.46
1:A:316:THR:O	1:A:320:VAL:HG23	2.15	0.46
1:A:390:LEU:HD13	1:A:530:VAL:HG22	1.96	0.46
1:A:588:GLY:O	1:A:600:MET:HB2	2.16	0.46
1:A:178:LEU:O	1:A:182:GLU:HG3	2.16	0.46
1:A:665:GLN:NE2	1:A:669:ASN:HD22	2.13	0.46
1:A:820:ILE:HD11	1:A:867:GLN:HB2	1.98	0.46
1:A:367:PHE:O	1:A:371:ASN:ND2	2.49	0.46
1:A:470:PHE:CZ	1:A:549:ILE:HG12	2.50	0.46
1:A:615:LEU:HD22	1:A:619:LEU:HG	1.98	0.46
1:A:636:ASP:HA	1:A:639:ASN:HD22	1.81	0.46
1:A:511:ASN:O	1:A:512:ALA:C	2.53	0.46
1:A:732:ARG:HH11	1:A:732:ARG:HB2	1.80	0.46
1:A:506:VAL:HG11	1:A:675:ARG:NH2	2.31	0.45
1:A:592:LEU:CD1	1:A:592:LEU:N	2.80	0.45
1:A:324:GLN:HB3	1:A:325:PRO:HD3	1.98	0.45
1:A:137:ARG:CG	1:A:137:ARG:NH1	2.80	0.45
1:A:363:GLU:OE2	1:A:516:ARG:HD3	2.17	0.45
1:A:43:LEU:HD23	1:A:97:TYR:CD2	2.52	0.45
1:A:494:GLN:NE2	1:A:494:GLN:HA	2.32	0.45
1:A:563:THR:O	1:A:567:ARG:HB2	2.17	0.45
1:A:671:ASP:O	1:A:674:VAL:HG12	2.17	0.45
1:A:78:PRO:O	1:A:80:ALA:N	2.49	0.45
1:A:95:ILE:HA	1:A:130:PHE:HE1	1.82	0.45
1:A:331:TYR:HD1	1:A:334:ILE:HD13	1.82	0.45
1:A:665:GLN:HE21	1:A:669:ASN:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:ARG:NH1	1:A:832:ARG:HG2	2.32	0.45
1:A:330:SER:OG	1:A:332:LYS:HG3	2.17	0.45
1:A:-2:PHE:O	1:A:2:THR:HG22	2.16	0.45
1:A:505:GLY:C	1:A:507:GLU:N	2.70	0.45
1:A:494:GLN:NE2	1:A:494:GLN:CA	2.80	0.44
1:A:626:GLU:HA	1:A:626:GLU:OE1	2.17	0.44
1:A:898:VAL:HG22	1:A:907:ILE:O	2.17	0.44
1:A:745:MET:HG3	1:A:802:LEU:HD12	2.00	0.44
1:A:755:ILE:N	1:A:756:PRO:HD3	2.33	0.44
1:A:782:PRO:O	1:A:786:GLU:HB2	2.18	0.44
1:A:40:ASP:CA	1:A:93:LEU:HD13	2.48	0.44
1:A:679:ARG:HH12	1:A:682:ASN:HD22	1.64	0.44
1:A:220:ILE:HA	1:A:223:LEU:HD22	2.00	0.44
1:A:11:THR:O	1:A:23:LEU:HD23	2.18	0.44
1:A:570:GLU:H	1:A:570:GLU:HG3	1.28	0.44
1:A:677:VAL:O	1:A:681:LEU:HB2	2.18	0.44
1:A:700:ASN:O	1:A:703:ASN:HB3	2.18	0.44
1:A:725:THR:O	1:A:729:SER:HB2	2.17	0.44
1:A:117:ILE:HG12	1:A:154:THR:CG2	2.47	0.44
1:A:420:LYS:HB2	1:A:420:LYS:HE3	1.87	0.44
1:A:590:MET:HA	1:A:591:PRO:HD3	1.88	0.44
1:A:655:ILE:HA	1:A:656:PRO:HD2	1.91	0.44
1:A:90:ILE:O	1:A:94:VAL:HG23	2.18	0.44
1:A:394:HIS:O	1:A:398:GLY:HA3	2.18	0.43
1:A:521:VAL:CB	1:A:522:PRO:CD	2.95	0.43
1:A:693:SER:O	1:A:696:ALA:HB3	2.18	0.43
1:A:900:LEU:HD21	1:A:912:ILE:HG21	2.00	0.43
1:A:357:LEU:HD13	1:A:528:GLU:HA	2.00	0.43
1:A:510:ASP:C	1:A:512:ALA:N	2.72	0.43
1:A:537:TYR:O	1:A:541:ILE:HG13	2.18	0.43
1:A:893:ILE:HD11	1:A:944:ILE:HG23	1.99	0.43
1:A:89:GLU:OE1	1:A:89:GLU:HA	2.18	0.43
1:A:208:PRO:HA	1:A:211:PHE:CE1	2.53	0.43
1:A:357:LEU:HD23	1:A:523:PHE:CE1	2.53	0.43
1:A:631:SER:O	1:A:632:SER:CB	2.66	0.43
1:A:555:LEU:HD22	1:A:559:VAL:HG23	2.01	0.43
1:A:511:ASN:HB3	1:A:515:LEU:HG	2.01	0.43
1:A:906:ASN:HD21	1:A:937:ASN:ND2	2.16	0.43
1:A:724:GLN:C	1:A:726:ARG:H	2.21	0.43
1:A:893:ILE:O	1:A:893:ILE:HG23	2.18	0.43
1:A:850:SER:CB	1:A:851:PRO:HA	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:VAL:HG23	3:A:1004:HOH:O	2.19	0.43
1:A:78:PRO:C	1:A:80:ALA:H	2.22	0.43
1:A:13:ASP:HA	1:A:14:PRO:HD3	1.87	0.42
1:A:520:PRO:HG3	1:A:571:LEU:HD22	2.00	0.42
1:A:466:GLN:HB3	1:A:548:PRO:CG	2.48	0.42
1:A:562:THR:HG23	1:A:581:LEU:HB3	2.01	0.42
1:A:404:GLU:CB	1:A:456:LEU:HD13	2.48	0.42
1:A:907:ILE:HD13	1:A:912:ILE:HG23	2.00	0.42
1:A:14:PRO:HA	1:A:22:LEU:CD1	2.47	0.42
1:A:567:ARG:O	1:A:569:PRO:HD3	2.18	0.42
1:A:765:VAL:HG13	1:A:766:TYR:N	2.35	0.42
1:A:837:ARG:CZ	1:A:837:ARG:HB3	2.49	0.42
1:A:624:ILE:C	1:A:626:GLU:H	2.23	0.42
1:A:315:ILE:HG22	1:A:319:LEU:HD22	2.01	0.42
1:A:721:LYS:CG	1:A:722:GLU:H	2.31	0.42
1:A:234:ASN:HB3	1:A:249:ILE:HD11	2.02	0.42
1:A:466:GLN:HB3	1:A:548:PRO:HG3	2.01	0.42
1:A:117:ILE:HD11	1:A:158:TYR:HB2	2.01	0.41
1:A:791:ASP:HB2	1:A:794:SER:OG	2.19	0.41
1:A:-1:ARG:C	1:A:2:THR:HG22	2.39	0.41
1:A:683:ASP:O	1:A:687:LEU:HG	2.19	0.41
1:A:804:LYS:NZ	1:A:849:ALA:H	2.18	0.41
1:A:92:ARG:NH1	1:A:93:LEU:HD21	2.36	0.41
1:A:46:GLN:O	1:A:53:LEU:HD12	2.20	0.41
1:A:357:LEU:HD12	1:A:357:LEU:HA	1.73	0.41
1:A:74:THR:CG2	1:A:80:ALA:HA	2.50	0.41
1:A:365:ASP:O	1:A:368:TYR:HB2	2.20	0.41
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.85	0.41
1:A:462:HIS:CD2	1:A:465:LEU:HG	2.55	0.41
1:A:47:LEU:HD11	1:A:60:LEU:HD21	2.03	0.41
1:A:640:SER:O	1:A:644:ILE:HG13	2.20	0.41
1:A:795:TYR:O	1:A:796:SER:HB2	2.20	0.41
1:A:850:SER:CB	1:A:851:PRO:CA	2.93	0.41
1:A:641:ARG:NH1	1:A:683:ASP:OD2	2.53	0.41
1:A:498:PRO:HG3	1:A:567:ARG:CZ	2.50	0.41
1:A:467:LEU:HD23	1:A:467:LEU:HA	1.91	0.41
1:A:541:ILE:HD12	1:A:542:SER:N	2.35	0.41
1:A:791:ASP:CB	1:A:794:SER:OG	2.69	0.41
1:A:238:ASN:ND2	1:A:240:LEU:H	2.19	0.41
1:A:732:ARG:CZ	1:A:732:ARG:CB	3.00	0.41
1:A:953:GLU:C	1:A:954:GLU:HG3	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:VAL:C	1:A:508:ASN:H	2.24	0.40
1:A:576:HIS:ND1	1:A:633:GLN:HG3	2.36	0.40
1:A:167:ASP:OD2	1:A:169:ASN:HB2	2.22	0.40
1:A:529:PHE:CD2	1:A:529:PHE:C	2.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	937/982 (95%)	848 (90%)	72 (8%)	17 (2%)	10	17

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	849	ALA
1	A	510	ASP
1	A	720	ASP
1	A	848	LEU
1	A	877	GLU
1	A	79	ASN
1	A	170	GLU
1	A	105	GLU
1	A	223	LEU
1	A	521	VAL
1	A	-4	SER
1	A	78	PRO
1	A	84	HIS
1	A	19	GLY
1	A	569	PRO
1	A	504	ILE
1	A	847	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	854/882 (97%)	781 (92%)	73 (8%)	12	22

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	GLU
1	A	-2	PHE
1	A	13	ASP
1	A	25	SER
1	A	27	GLU
1	A	41	THR
1	A	51	GLU
1	A	54	ASP
1	A	65	ARG
1	A	81	GLU
1	A	114	ILE
1	A	123	ASN
1	A	137	ARG
1	A	139	ILE
1	A	141	GLU
1	A	147	LEU
1	A	151	VAL
1	A	180	ILE
1	A	181	PHE
1	A	193	ILE
1	A	209	GLN
1	A	215	THR
1	A	217	LEU
1	A	223	LEU
1	A	238	ASN
1	A	249	ILE
1	A	253	LEU
1	A	258	LYS
1	A	264	LEU
1	A	270	LYS

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Mol	Chain	Res	Type
1	A	277	ASN
1	A	297	ARG
1	A	317	LEU
1	A	318	LEU
1	A	319	LEU
1	A	327	LEU
1	A	357	LEU
1	A	373	LYS
1	A	393	LEU
1	A	404	GLU
1	A	418	ILE
1	A	494	GLN
1	A	497	LEU
1	A	551	ARG
1	A	555	LEU
1	A	566	LEU
1	A	567	ARG
1	A	570	GLU
1	A	582	VAL
1	A	585	LEU
1	A	594	ASP
1	A	614	LEU
1	A	615	LEU
1	A	625	VAL
1	A	633	GLN
1	A	636	ASP
1	A	648	LEU
1	A	677	VAL
1	A	679	ARG
1	A	719	GLU
1	A	733	GLN
1	A	740	LEU
1	A	742	ASP
1	A	750	ILE
1	A	820	ILE
1	A	858	LEU
1	A	859	ASN
1	A	912	ILE
1	A	925	ASN
1	A	926	ARG
1	A	932	GLU
1	A	935	THR

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Mol	Chain	Res	Type
1	A	954	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	61	ASN
1	A	68	GLN
1	A	76	ASN
1	A	103	GLN
1	A	136	GLN
1	A	175	ASN
1	A	209	GLN
1	A	234	ASN
1	A	238	ASN
1	A	250	HIS
1	A	293	ASN
1	A	314	ASN
1	A	380	ASN
1	A	394	HIS
1	A	438	GLN
1	A	462	HIS
1	A	494	GLN
1	A	508	ASN
1	A	639	ASN
1	A	661	GLN
1	A	665	GLN
1	A	667	GLN
1	A	702	GLN
1	A	724	GLN
1	A	773	ASN
1	A	775	ASN
1	A	798	ASN
1	A	812	ASN
1	A	816	GLN
1	A	831	ASN
1	A	906	ASN
1	A	915	HIS
1	A	925	ASN
1	A	942	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	943/982 (96%)	0.10	30 (3%)	48 45	35, 56, 106, 136	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	634	PHE	7.2
1	A	506	VAL	6.1
1	A	38	PHE	6.0
1	A	504	ILE	5.7
1	A	631	SER	4.9
1	A	632	SER	4.8
1	A	10	ILE	4.7
1	A	635	TYR	4.2
1	A	703	ASN	3.9
1	A	521	VAL	3.7
1	A	24	LYS	3.5
1	A	-1	ARG	3.5
1	A	11	THR	3.5
1	A	377	SER	3.0
1	A	848	LEU	3.0
1	A	18	ARG	2.9
1	A	23	LEU	2.8
1	A	951	LYS	2.8
1	A	721	LYS	2.5
1	A	858	LEU	2.5
1	A	880	ASP	2.4
1	A	593	THR	2.4
1	A	630	SER	2.3
1	A	507	GLU	2.2
1	A	629	GLY	2.2
1	A	-2	PHE	2.2
1	A	509	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	947	PHE	2.1
1	A	-3	GLU	2.1
1	A	945	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	K	A	962	1/1	0.97	0.11	-	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.